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CONFIDENCE BOUNDS FOR THE LINEAR
MODEL OF LESS THAN THE FULL RANK
WITH AN INTRODUCTION TO G-INVERSES

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I. INTRODUCTION

While Grubbs¹ discusses linear statistical regression and functional relations in a general way in BRL Report No. 1842, Taylor and Moore² explain in BRL Report No. 1986 the use of Scheffé's theorem³ in providing simultaneous confidence bounds for a polynomial in the set-up of a general linear hypothesis model where the design matrix X is of full rank. The aim of the first report was, as it appears, to provide an introduction to the subject of linear regression and that of the second, to make Scheffé's theorem³ accessible to the general reader in the set-up of a nonsingular design matrix X . In this context, one may also like to know how Scheffé's theorem could be used when the design matrix is singular. This is important, since most of the Experimental Design Models are characterized by singular matrices. In the perspective of using Scheffé's theorem when the design matrix X is singular, it may also be of interest to know how the basic results under the general linear hypothesis model of full rank would extend to the situation when the design matrix X is singular. With this objective in mind, some of the relevant results which are very basic in the theory of singular designs are brought together in this report paving the background with an explanatory introduction to the solution of linear equations as related to the concept of a generalized inverse (g-inverse).

II. THE GENERAL LINEAR HYPOTHESIS MODEL OF FULL RANK

A. Characterization of the Linear Model

Suppose a set of $(p-1)$ mathematical variables, x_1, x_2, \dots, x_{p-1} are related to a random variable y which is observed with an unknown random error ϵ in the following manner,

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_{p-1} x_{p-1} + \epsilon \quad (1)$$

¹Grubbs, F. E., "Linear Statistical Regression and Functional Relations," Ballistic Research Lab Report No. 1842, AD #A018651, 1975.

²Taylor, M.S., and Moore, J.R., "Confidence Bounds for the General Linear Model," Ballistic Research Lab Report No. 1986, 1977. (AD#A041035)

³Scheffé, H., "The Analysis of Variance," John Wiley & Sons, Inc., New York, 1959.

where β_j ($j = 0, 1, 2, \dots, p-1$) are unknown parameters (constants). Equation (1), which is linear in the random variables, y and ϵ , and the parameters, $\beta_0, \beta_1, \dots, \beta_{p-1}$, represents a linear model. When all the observations are taken in accordance with this model, observing a y for each set of the x 's, the observational equations are expressible in matrix notation as

$$\underline{y} = X \underline{\beta} + \underline{\epsilon} \quad (2)$$

With n observations, \underline{y} is an $n \times 1$ column vector of the observed y 's, $X = (x_{ij})$, ($i = 1, 2, 3, \dots, n$, $j = 0, 1, 2, \dots, p-1$), is a known $n \times p$ matrix with x_{ij} as its (i, j) th element; $\underline{\beta}$ is a $p \times 1$ vector of unknown parameters, β_j ($j = 0, 1, 2, \dots, p-1$); $\underline{\epsilon}$ is an $n \times 1$ vector of unobserved random errors, ϵ_i ($i = 1, 2, 3, \dots, n$).

When $\text{Rank}(X) = p$, we say that the model is of full rank. In the analysis of such models we usually consider the following two cases concerning the distribution of $\underline{\epsilon}$.

Case 1: $\underline{\epsilon}$ is distributed normally with mean $\underline{0}$ and covariance $\sigma^2 I$, $\sigma^2 > 0$, where I is the $n \times n$ identity matrix. (These assumptions are needed for tests of hypothesis and setting confidence bounds.)

Case 2: $\underline{\epsilon}$ has an unknown distribution with mean $\underline{0}$ and covariance $\sigma^2 I$. (These assumptions are referred to as the "Least Squares" assumptions.)

B. Some of the Basic Results Relevant to the Full Rank Model

The normal equations to provide the least squares point estimate $\hat{\underline{\beta}}$ of $\underline{\beta}$ are given by

$$(X'X)\hat{\underline{\beta}} = X'\underline{y} \quad (3)$$

$$\Rightarrow \hat{\underline{\beta}} = (X'X)^{-1}X'\underline{y} \quad (4)$$

The equations to provide the maximum likelihood estimate of $\underline{\beta}$ for Case 1 will be the same. The least squares point estimate $\hat{\sigma}^2$ of σ^2 (the same for maximum likelihood estimate, when adjusted for bias) is given by

$$\hat{\sigma}^2 = \frac{1}{n-p} (\underline{y} - X\hat{\underline{\beta}})' (\underline{y} - X\hat{\underline{\beta}}) = \frac{1}{n-p} [\underline{y}'\underline{y} - \hat{\underline{\beta}}'X'\underline{y}] \quad (5)$$

The estimates $\hat{\underline{\beta}}$ and $\hat{\sigma}^2$ are unbiased. That is $E(\hat{\underline{\beta}}) = \underline{\beta}$, $E(\hat{\sigma}^2) = \sigma^2$, where the symbol E stands for mathematical expectation. The least squares

estimate $\underline{\hat{\beta}}$ of $\underline{\beta}$, where $\underline{\ell}$ is any $p \times 1$ vector of constants, is given by

$$\underline{\hat{\beta}} = \underline{\ell}' (X'X)^{-1} X'y \quad (6)$$

and the variance of $\underline{\hat{\beta}}$ by

$$\text{Var} (\underline{\hat{\beta}}) = \sigma^2 \underline{\ell}' (X'X)^{-1} \underline{\ell} \quad (7)$$

In particular, $\underline{\ell}'$ may be any given observation vector $(1, x_1, \dots, x_{p-1})$. Under the assumptions of Case 1, $\underline{\hat{\beta}}$ has the multivariate normal distribution with mean $\underline{\beta}$, and variance $\sigma^2 S^{-1}$, where $S = (X'X)$.

C. Estimation of a Parametric Function When the Design Matrix is Singular

When the design matrix X is of full rank, that is, when $\text{Rank}(X) = p$, we can provide, as noted above, an estimate for each element of $\underline{\beta}$, and therefore, also an estimate $\underline{\ell}'\underline{\hat{\beta}}$ for $\underline{\ell}'\underline{\beta}$, for any $p \times 1$ vector $\underline{\ell}$. However, when the design matrix X is not of full rank, that is, when $\text{Rank}(X) = r$, $r < p$, implying that $\text{Rank}(X'X) = r$, we cannot provide unique solutions to the normal equations (3). Unique solutions given in (4) require a regular inverse of $(X'X)$. Since $(X'X)$ is not of full rank, we cannot compute a regular inverse. None-the-less, the normal equations (3) can still be solved, and some of the results given in the preceding section can still be obtained in analogous forms by using what is called a generalized inverse (g-inverse or a pseudo-inverse) of the matrix $(X'X)$. In order to make this report self-contained, we provide in the sequel an elementary introduction to the solution of numerical equations as related to the concept of a "generalized inverse" (g-inverse).

When the model is of less than the full rank, we can provide unbiased estimates of some specific linear functions of the parameters. Such functions are called estimable functions. This brings in the definition of estimability.

A linear parametric function, $\psi = \underline{c}'\underline{\beta} = c_1\beta_1 + c_2\beta_2 + \dots + c_p\beta_p$, is said to be estimable, if and only if it has an unbiased linear estimate $\underline{\hat{\psi}}$. That is, there should exist an $n \times 1$ vector \underline{a} , such that $E(\underline{\hat{\psi}}) = E(\underline{a}'y) = \psi$, which in turn implies that $\underline{a}'X\underline{\beta} = \underline{c}'\underline{\beta}$, for all $\underline{\beta}$. Hence, \underline{c}' should be of the form $\underline{a}'X$ which is a row vector in the row space of X .

D. Scheffé's Theorem

We note here again that all linear parametric functions are uniquely estimable in the full rank model. In such a situation, we can think of p independent linear functions of the parameters given as $\psi_1, \psi_2, \dots, \psi_p$,

forming what may be called a basis of the p -dimensional space L of the parametric functions. Thus, in the full rank model under Case 1, Scheffé's theorem on simultaneous confidence bounds will read as follows:

Theorem 1: The probability is $1-\alpha$ (where α is the size of the associated test of hypothesis) that the values of all parametric functions $\psi \in L$ simultaneously satisfy the inequalities:

$$\hat{\psi} - S\hat{\sigma}_{\hat{\psi}} \leq \psi \leq \hat{\psi} + S\hat{\sigma}_{\hat{\psi}}, \quad (8)$$

where $S^2 = [pF_{\alpha}; p, n-p]$, F denoting Snedecor's F distribution with p and $(n-p)$ degrees of freedom, and $\hat{\sigma}_{\hat{\psi}}$ is the estimated standard error of $\hat{\psi}$.

If one is interested in a set of q ($q < p$) independent parametric functions, $\underline{\psi}' = (\psi_1, \dots, \psi_q)$, S^2 will change to $[qF_{\alpha}; q, n-p]$, making the confidence interval shorter.

The likelihood ratio test which provides the simultaneous confidence bounds (8) for ψ provides simultaneous bounds also on all linear combinations of ψ_i ($i = 1, 2, \dots, q$), $\underline{l}'\underline{\psi} = \phi$, where \underline{l} is any $q \times 1$ column vector of constants (see [3,8]). The corresponding theorem on confidence bounds will then read as follows:

Theorem 2: The probability is $1-\alpha$ (where α is the size of the associated test of hypothesis) that the values of all possible linear combinations, ϕ , of the linear parametric functions simultaneously satisfy the inequalities:

$$\hat{\phi} - S\hat{\sigma}_{\hat{\phi}} \leq \phi \leq \hat{\phi} + S\hat{\sigma}_{\hat{\phi}} \quad (9)$$

where $S^2 = [qF_{\alpha}; q, n-p]$.

In order to apply Scheffé's theorem in the context of a singular model, we need the following introduction to the solution of a system of linear equations as related to the concept and computation of the generalized inverse (g -inverse) of a matrix.

III. ON THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS

A. Necessary Operations Required to Solve Linear Equations with a Singular Coefficient Matrix.

A system of n linear equations in n unknowns may be written as

$$\underline{Ax} = \underline{y} \quad (10)$$

where the coefficient matrix A is an $n \times n$ matrix of known constants, \underline{x} is a $n \times 1$ vector of the unknown variables, and \underline{y} is a vector of known constants.

When $\text{Rank}(A) = n$, the solution of the equations is obtained as $\underline{x} = A^{-1}\underline{y}$.

When $\text{Rank}(A) = p < n$, A^{-1} does not exist. But the system of equations may still have a solution, when the equations are consistent. Solutions for such a system of equations exist, when and only when $\text{Rank}(A) = \text{Rank}(A:\underline{y})$, which, in turn, implies that \underline{y} lies in the column space of A . This provides, in fact, also the condition for consistency of the equations.

In the general situation, the matrix A need not be a square matrix.

$\underline{Ax} = \underline{0}$ of equation (10) will be referred to as the homogeneous part of the system. As we know, to solve a system of equations, any one equation can be multiplied or divided by a constant (other than 0), and that any two equations may be added, or one equation may be subtracted from another without affecting the solutions. These operations on the equations may be performed by the appropriate operations on the rows of A and the corresponding elements of \underline{y} .

By premultiplying a given matrix by what is called an elementary matrix E , we can interchange any two rows, multiply a row by a non-zero scalar, or replace the i th row by the sum of the i th row and c times the j th row. These elementary matrices are obtained from the identity matrices of appropriate dimensions after performing corresponding operations on the identity matrices. Let us suppose that A is of dimension 3×3 . The elementary matrices will then be obtained from the identity matrix I_3 of dimension 3.

The elementary matrix E_{12} to interchange the first and second row of A will be given by

$$E_{12} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

E_{12} is obtained by interchanging the first and the second row of I_3 .

The elementary matrix to multiply the second row of A by 3 will be given by

$$E_2(3) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix} .$$

$E_2(3)$ is obtained by multiplying the second row of I_3 by 3.

The elementary matrix to replace the second row of A by the sum of the second row and (-3) times the third row will be given by

$$E_{23}(-3) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -3 \\ 0 & 0 & 1 \end{bmatrix} .$$

$E_{23}(-3)$ is obtained by replacing the second row of I_3 by the sum of the second row and (-3) times the third row of I_3 .

If A is a $p \times p$ nonsingular matrix, we can reduce A to the identity matrix I_p by a finite number (say, t) of row operations on A. That is,

$$\begin{aligned} E_t E_{t-1} \dots E_1 A &= I_p \\ \Rightarrow E_t E_{t-1} \dots E_1 &= A^{-1} . \end{aligned}$$

It is then observed that the product of the elementary matrices gives the inverse of A, when A is nonsingular.

It may be pointed out that post-multiplication by the elementary matrices E obtained from the column operations on the identity matrix provides the corresponding column operations.

B. A Numerical Illustration of Solving a System of Linear Equations by the Sweep-out Method.

Given below is a system of 3 linear equations in 4 variables. Here, the associated coefficient matrix A has 3 rows and 4 columns.

(1). Equations: $x_1 + 2x_2 + 3x_3 + x_4 = 4$

$4x_1 + 5x_2 + 6x_3 + 2x_4 = 5$

$8x_1 + 13x_2 + 18x_3 + 6x_4 = 21$

Homogeneous part

Non-homogeneous part

$x_1 + 2x_2 + 3x_3 + x_4 = 0$ = 4

$4x_1 + 5x_2 + 6x_3 + 2x_4 = 0$ = 5

$8x_1 + 13x_2 + 18x_3 + 6x_4 = 0$ = 21

$E_{32}(-1), E_{31}(-4)$

1 2 3 1 = 4

4 5 6 2 = 5

0 0 0 0 = 0

$E_{21}(-4)$

1 2 3 1 = 4

0 -3 -6 -2 = -11

0 0 0 0 = 0

$E_2(-1)$

1 2 3 1 = 4

0 3 6 2 = 11

0 0 0 0 = 0

$E_2(1/3)$

1 2 3 1 = 4

0 1 2 2/3 = 11/3

0 0 0 0 = 0

$E_{12}(-2)$

1 0 -1 -1/3 = -10/3

0 1 2 2/3 = 11/3

0 0 0 0 = 0

The method of elimination adopted above is sometimes referred to in literature as the method of "sweep-out." The method of "sweep-out" gives us a basis of the row space of A along with the solutions, if solutions exist. Solutions will exist, if when a row is swept out leaving 0's as its elements, the corresponding element of \underline{y} should also go to 0 in the "sweep-out" procedure. The "sweep-out" procedure, therefore, gives us also a way of finding if the equations are consistent.

The third row has been swept out, retaining only two equations in four variables. The first row could have been swept out, and the last two rows raised above, retaining the same form of the reduced coefficient matrix. The form is important. It may be pointed out that other kinds of row operations could also have been performed, retaining the same form of the reduced coefficient matrix. Now, merely from an inspection of the non-zero part of the reduced coefficient matrix, it is possible to find a solution vector of the homogeneous part, a vector that is orthogonal to a row of the reduced matrix. Such solutions are indicated below.

(2). Solutions of the Homogeneous Part

		Solutions shown as columns										
Basis	{	[1	0	-1	-1/3]		[-1	-1/3]
			0	1	2	2/3				2	2/3	
											
Solns. shown as rows	{	[-1	2	-1	0]		[-1	0]
	⇒		-1/3	2/3	0	-1				0	-1	

(3). A Particular Solution of the Equations $A\underline{x} = \underline{y}$

$$\begin{array}{l} x_1 = -10/3 \\ x_2 = 11/3 \\ x_3 = 0 \\ x_4 = 0 \end{array} .$$

This comes from the nonhomogeneous part, and is obtained by adding two zeros to the reduced part of the vector \underline{y} . If there are four equations in two variables, we can assign arbitrary values to two of the variables, and solve uniquely for the remaining two variables. In this case, zero values are assigned to the third and the fourth variables.

(4).

General Solution

Particular Solution

+

General Solution from the homogeneous part

$$\begin{array}{l} x_1 = \\ x_2 = \\ x_3 = \\ x_4 = \end{array} \begin{bmatrix} -10/3 \\ 11/3 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} \lambda \begin{pmatrix} -1 \\ 2 \\ -1 \\ 0 \end{pmatrix} + \mu \begin{pmatrix} -1/3 \\ 2/3 \\ 0 \\ -1 \end{pmatrix} \end{bmatrix},$$

λ, μ being arbitrary scalars.

It should not be difficult to verify how all possible solutions are included in the above general solution. Suppose we want to find the values of x_1 and x_2 by assigning c_1 to x_3 , c_2 to x_4 , instead of 0's. This solution will then be given by writing $\lambda = -c_1$, and $\mu = -c_2$.

Each step taken in the elimination process shown above is equivalent to an elementary row operation provided by premultiplication with elementary matrices, $E_{ij}(c)$, $E_i(k)$, etc. These elementary matrices are indicated prior to the steps taken.

If necessary, a row of 0's may be added to make the matrix A square (i.e. 4x4). Correspondingly, the vector \underline{y} may be made to consist of 4 elements, with the fourth element as zero.

Writing B as the product of the elementary matrices required to reduce A to the standard form, it is obtained as

$$B = E_{12}(-2) E_2(1/3) E_2(-1) E_{21}(-4) E_{32}(-1) E_{31}(-4) I_4$$

$$= \begin{bmatrix} -5/3 & 2/3 & 0 & 0 \\ 4/3 & -1/3 & 0 & 0 \\ -4 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

where A is of dimension 4x4.

One may also introduce "economy" in the number of row operations or perform other row operations and get a different form for B. B has been obtained the same way as a regular inverse of A is sometimes obtained, when A is nonsingular. $B = A^{-1}$ is unique, when A is nonsingular. But, B is not unique, when A is singular. Other forms of B could be found⁴ reducing A to the above standard form.

It may be verified that the particular solution, referred to above, is given by $\underline{B}\underline{y}$. In this case, the last column of B is redundant, as it does not contribute to the solution. The last column of B has a unity in the fourth row, while the rest of the elements are 0's, and \underline{y} has a 0 in the fourth row. Omitting the fourth column of B, the remaining 4x3 matrix can be taken as a g-inverse of A. Calling it B, a solution for \underline{x} is given by $\underline{x} = \underline{B}\underline{y}$.

Although B is not unique, the particular solution $\underline{B}\underline{y}$ has a unique character. It should be evident that the values of x_1 and x_2 come from

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 4 & 5 \end{bmatrix}^{-1} \begin{bmatrix} 4 \\ 5 \end{bmatrix}.$$

The values of x_1 and x_2 are unique. If, for example, the first row were swept out, retaining the second and the third rows, the values of x_1 and x_2 would have come from

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 4 & 5 \\ 8 & 13 \end{bmatrix}^{-1} \begin{bmatrix} 5 \\ 21 \end{bmatrix}.$$

The values of x_1 and x_2 are the same as above. In both cases, x_3 and x_4 are assigned zero values. (This aspect of uniqueness of $\underline{B}\underline{y}$ is referred to later in this report.)

C. The General Solution in a Compact Form

The general solution to the equations $A\underline{x} = \underline{y}$ can be written in a compact form as

$$\underline{x} = \underline{B}\underline{y} + (\underline{H}-\underline{I})\underline{z}, \quad (11)$$

where $\underline{H} = \underline{B}\underline{A}$, and \underline{z} is any arbitrary vector. The first part of the

⁴Banerjee, K.S., "Singularity in Hotelling's Weighing Designs and a Generalized Inverse," Annals of Math. Stat., 37, 4, 1021-31 (1966). (Correction note: Annals of Math. Stat., 40, 2, 719.)

solution, $\underline{B}\underline{y}$, is what has been termed as the particular solution, while the second component is derived from the homogeneous part. As \underline{z} is arbitrary, the above solutions may also be expressed as $\underline{B}\underline{y} + (\underline{I}-\underline{H})\underline{z}$. We may adopt any one of these two forms. We provide below a derivation of the compact form of the general solution by way of summarizing what has been done under the "sweep-out" operations.

D. The Derivation of the General Solution

The second component of the general solution comes from the homogeneous part. We recall that a matrix \underline{B} exists such that $\underline{B}\underline{A} = \underline{H}$ where \underline{H} is of a particular form. That is,

$$\underline{A}\underline{x} = \underline{0} \Rightarrow \underline{H}\underline{x} = \underline{0}$$

$$\Rightarrow \left[\begin{array}{c|c} \underline{I}_p & \underline{H}_{12} \\ \hline 0 & 0 \end{array} \right] \underline{x} = \underline{0} \Rightarrow \text{The solutions are given by}$$

$$\left[\begin{array}{c} \underline{H}_{12} \\ \hline -\underline{I}_{n-p} \end{array} \right] \underline{z}_{n-p} \quad (12)$$

Any column in the column space of (12) is also a solution. That is,

$$\left[\begin{array}{c} \underline{H}_{12} \\ \hline -\underline{I}_{n-p} \end{array} \right] \underline{z}_{n-p}$$

is also a solution, where \underline{z}_{n-p} is a vector of $(n-p)$ elements. Also,

$$\left[\begin{array}{c|c} 0_{p \times p} & \underline{H}_{12} \\ \hline 0_{(n-p) \times p} & -\underline{I}_{n-p} \end{array} \right] \left[\begin{array}{c} \underline{z}_p \\ \hline \underline{z}_{n-p} \end{array} \right] = (\underline{H}-\underline{I})\underline{z}$$

is a solution, where \underline{z} is arbitrary. Introduction of \underline{z}_p adds 0 to the solution. It may be noted that this whole part merely adds 0 to the R.H.S. of the equations, $\underline{A}\underline{x} = \underline{y}$.

The first component, $\underline{B}\underline{y}$, of the general solution, called a particular solution, comes as follows:

$$A\underline{x} = \underline{y}$$

$$\Rightarrow \begin{bmatrix} I_p & H_{12} \\ \hline 0 & 0 \end{bmatrix} \underline{x} = B\underline{y} = \begin{bmatrix} \underline{y}_p \\ \hline 0_{n-p} \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} I_p & H_{12} \\ \hline 0 & 0 \end{bmatrix} \begin{bmatrix} \underline{x}_p \\ \hline \underline{x}_{n-p} \end{bmatrix} = \begin{bmatrix} \underline{y}_p \\ \hline 0_{n-p} \end{bmatrix} \quad (13)$$

where the suffixes attached to the column vectors indicate their dimensions. (13) implies that

$$\underline{x}_p = \underline{y}_p - H_{12}\underline{x}_{n-p}$$

Since we can assign arbitrary values to the elements of the vector \underline{x}_{n-p} , we can set it to 0 to get a solution. This solution has been termed the particular solution, being given by

$$\begin{bmatrix} \underline{x}_p \\ \hline \underline{x}_{n-p} \end{bmatrix} = \begin{bmatrix} \underline{y}_p \\ \hline 0_{n-p} \end{bmatrix} = B\underline{y}.$$

Combining the two together, we get the general solution in the above form.

IV. GENERALIZED INVERSES

A. Introductory Remarks

It has been observed in the preceding sections that even when the rank of the coefficient matrix A is less than the full, we can find solutions to the system of equations, $A\underline{x} = \underline{y}$, when the equations are consistent. It has also been observed that $B\underline{y}$ gives a solution, (a particular one), which is a component part of the general solution. Thus, B takes the place of the inverse of A , and may, therefore, be taken as a pseudo-inverse or, more generally, as a generalized inverse (g-inverse) of A . Some authors designate an inverse such as B as a conditional inverse. There are, in fact, many other pseudo-inverses, or generalized inverses (g-inverses) depending on the properties these inverses satisfy. All of these generalized inverses are not unique, as we have shown for B . Only one of these inverses, the one due to Moore-Penrose, is unique. For this unique g-inverse, we shall reserve the symbol "+", while for other g-inverses, we shall use "-".

The following is an introduction to g-inverses. The material for the first part of this discussion is drawn from Rao⁵, while that for the second part from Greville.⁶ One may refer to these two references and also to Price⁷, Graybill⁸ and Banerjee⁴ for details and further insight.

B. A G-inverse That is Not Unique. (See C. R. Rao⁵)

Definition of g-inverse

A generalized inverse (or g-inverse) of a matrix A of order $m \times n$ is a matrix of order $n \times m$, denoted A^- , such that for any \underline{y} for which $A\underline{x} = \underline{y}$ is consistent, $\underline{x} = A^-\underline{y}$ is a solution.

Lemma 1. If A^- is a g-inverse, then $AA^-A = A$, and conversely.

Choose \underline{y} as the i^{th} column \underline{a}_i of A . Then, the equation $A\underline{x} = \underline{a}_i$ is consistent, as \underline{a}_i lies in the column space of A . Hence, $\underline{x} = A^-\underline{a}_i$ is a solution. That is, $AA^-\underline{a}_i = \underline{a}_i$, for all columns \underline{a}_i of A . This implies that $AA^-A = A$. Conversely, if A^- exists such that $AA^-A = A$, and $A\underline{x} = \underline{y}$ is consistent, then $AA^-A\underline{x} = A\underline{x} = \underline{y}$, or $AA^-\underline{y} = \underline{y}$. Hence, $A^-\underline{y}$ is a solution for $A\underline{x} = \underline{y}$. Thus, A^- is, by definition, a g-inverse.

Lemma 2. Let $AA^- = H$ for a given g-inverse A^- . Then

(a). $H^2 = H$; i.e., H is idempotent;

(b). $AH = A$.

Proof of (a): $H^2 = A^-AA^-A = A^-A = H$

Proof of (b): $AH = AA^-A = A$

⁵Rao, C.R., "A Note on a Generalized Inverse of a Matrix with Applications to Problems in Mathematical Statistics," J. Roy. Statist. Soc., B, 24, 152-158, 1962.

⁶Greville, T.N.E., "The Pseudo Inverse of a Rectangular or Singular Matrix and its Application to the Solution of Systems of Linear Equations," SIAM Review, Vol. 1, No. 1, pp. 38-43, Jan. 1959.

⁷Price, C. M., "The Matrix Pseudo Inverse and Minimal Variance Estimates," SIAM Review, Vol. 6, No. 2, 115-20, 1964.

⁸Graybill, F. A., "Theory and Application of the Linear Model," Duxbury Press, Massachusetts, 1976.

Lemma 3. A g-inverse exists for any matrix A, although it may not be unique, and it can be constructed in such a way that it has A itself as a g-inverse. In other words, it is possible to find A^- such that $AA^-A = A$, and that $A^-AA^- = A^-$.

Given a matrix A of order $m \times n$ and rank s, there exist non-singular matrices P and Q of orders m and n respectively, such that $PAQ = \Delta$, or $A = P^{-1}\Delta Q^{-1}$, where

$$\Delta = \left[\begin{array}{c|c} D & 0 \\ \hline 0 & 0 \end{array} \right],$$

and D_s is a diagonal matrix of order s and rank s. Let us define $A^- = Q\Delta^-P$, where

$$\Delta^- = \left[\begin{array}{c|c} D^{-1} & 0 \\ \hline 0 & 0 \end{array} \right].$$

This A^- satisfies

$$(a). AA^-A = A$$

$$(b). A^-AA^- = A^-.$$

Remark: If, in particular, A is a symmetric matrix, then $Q = P'$. It may also be pointed out the matrix P or Q can be obtained as a product of the elementary matrices introduced earlier.

Observation: In order that that A^- be unique, A^- has to satisfy, it is known^{6,7}, the following two additional relationships:

$$(c). (AA^-)' = AA^-$$

$$(d). (A^-A)' = A^-A.$$

C. The Unique G-inverse (See T. N. E. Greville⁶)

For any matrix A, there exists, as referred to above, a unique g-inverse A^+ such that

1. $A A^{\dagger} A = A$
2. $A^{\dagger} A A^{\dagger} = A^{\dagger}$
3. $(A A^{\dagger})' = A A^{\dagger}$
4. $(A^{\dagger} A)' = A^{\dagger} A$

D. Unique G-inverse for Special Rectangular Matrices B and C

1. If any matrix B is of dimensions $n \times m$, ($m \leq n$), and of rank m, then B^{\dagger} is obtained as

$$B^{\dagger} = (B' B)^{-1} B' . \quad (14)$$

2. If any matrix C is of dimensions $m \times n$ ($m \leq n$), and of rank m, then C^{\dagger} is obtained as

$$C^{\dagger} = C' (C C')^{-1} . \quad (15)$$

E. Left and Right Identity Matrices for any General Matrix A.

Let Rank (A) = $r < m$, and let B denote a matrix of r columns whose columns form a basis for the column space of A. [In particular, B might be formed by selecting r linearly independent columns of A.] Also, let C be an r-rowed matrix whose rows form a basis for the row space of A. [C may be formed by selecting r linearly independent rows of A.] The g-inverses of B and C are given by (14) and (15) above. Then A has a unique left identity I_L and a unique right identity I_R being given by

$$I_L = B B^{\dagger}$$

$$I_R = C^{\dagger} C,$$

such that $I_L A = A$, and $A I_R = A$. The proof follows from the fact that each column of A is a linear combination of the columns of B, and that each row of A is a linear combination of the rows of C.

F. Existence of a Unique G-inverse of a General Matrix

1. An Observation: For any matrix A, there is a unique matrix A^{\dagger} , which has its rows and columns in the row space and column space of A, and also satisfies the equations,

$$A A^{\dagger} = I_L, \quad \text{and} \quad A^{\dagger} A = I_R.$$

It can be verified that for B and C, the matrices B^\dagger and C^\dagger satisfy the above requirements.

2. A^\dagger in General. To get A^\dagger in general, we introduce the matrix G being given by

$$G = B^\dagger A C^\dagger .$$

From the above,

$$B G C = A .$$

It may be noted that G is of rank r. We finally define A^\dagger as

$$A^\dagger = C^\dagger G^{-1} B^\dagger .$$

(See Greville⁶ for uniqueness of A^\dagger .)

V. LINEAR HYPOTHESIS MODEL OF LESS THAN THE FULL RANK

A. The Problem of Estimation

The general linear hypothesis model introduced in equation (2) is of full rank, where $\text{Rank}(X) = p$. The model will be said to be of less than the full rank, when $\text{Rank}(X) = r < p$. Most of the problems in Design of Experiments are characterized by models of less than the full rank. Both under Case 1 (permitting the maximum likelihood estimation procedure) and under Case 2 (giving the least squares estimates) the normal equations are obtained as

$$(X'X)\hat{\underline{\beta}} = X'\underline{y} . \quad (16)$$

Since $\text{Rank}(X) = r$, $r < p$, Rank of $[X'X]$ is also r. Hence $(X'X)^{-1}$ does not exist, as $X'X$ is of dimension $p \times p$. However, we can still solve the equations using the first g-inverse of $X'X = S$ introduced earlier, and express the general solution for $\hat{\underline{\beta}}$ as

$$\hat{\underline{\beta}} = S^-X'\underline{y} + (I-H)\underline{z} \quad (17)$$

where $H = S^-S$.

The least squares estimate $\hat{\sigma}^2$ of σ^2 , and the maximum likelihood estimate $\hat{\sigma}^2$ of σ^2 (adjusted for the bias) are the same, being given by

$$\hat{\sigma}^2 = \frac{1}{n-r} [(\underline{y}-X\hat{\underline{\beta}})'(\underline{y}-X\hat{\underline{\beta}})] = \frac{1}{n-r} [\underline{y}'\underline{y} - \hat{\underline{\beta}}'X'\underline{y}] \quad (18)$$

where $\hat{\underline{\beta}}$ represents any solution of equation (16) given above in (17).

Since $\text{Rank}(S) = r$, it is not possible to provide a unique estimate for each element of $\underline{\beta}$. However, it is possible to provide a best (in the sense of minimum variance) and unbiased estimate of an estimable linear function of the elements of $\underline{\beta}$. It should be pointed out that all possible linear functions of the elements of $\underline{\beta}$ are not estimable. If it were so, every element of $\underline{\beta}$ would have been estimable. There are many equivalent, necessary and sufficient, conditions that would make a linear function of the parameters such as $\underline{\lambda}'\underline{\beta}$ (where $\underline{\lambda}'$ is a row vector of constants) estimable. We provide below a few of such necessary and sufficient conditions. For further details, one may refer to Graybill⁸.

A linear combination of the parameters, $\underline{\lambda}'\underline{\beta}$, is estimable, if and only if:

1. $\underline{\lambda}'$ is a row vector of X , or a linear combination of the row vectors of X . In other words, $\underline{\lambda}'$ is in the row space of X .
2. The equations $S\underline{r} = \underline{\lambda}$ are consistent, where $S = X'X$. That is, a solution \underline{r} exists for the equations.
3. $\underline{\lambda}'$ is of the form $\underline{\lambda}' = \underline{\lambda}'H$, where $H = S^-S$, and S^- is the first g-inverse of $S = X'X$, that is, the g-inverse that satisfies only the condition $SS^-S = S$.

B. On the Estimate, $\underline{\lambda}'\hat{\underline{\beta}}$

Although the normal equations (16) will have infinitely many solutions for $\hat{\underline{\beta}}$ implying that $\underline{\beta}$ is not unique, the estimate $\underline{\lambda}'\hat{\underline{\beta}}$ of the estimable function $\underline{\lambda}'\underline{\beta}$ is unique. Also, $\underline{\lambda}'\hat{\underline{\beta}}$ is unbiased, which can be shown using the first g-inverse which is more general than the unique g-inverse.

$$\begin{aligned}
 1. \text{ Unbiased: } E[\underline{\lambda}'\hat{\underline{\beta}}] &= E[\underline{\lambda}'(S^-X'\underline{y} + (I-H)\underline{z})] \\
 &= E[\underline{\lambda}'S^-X'\underline{y} + (\underline{\lambda}' - \underline{\lambda}'H)\underline{z}] \\
 &= E[\underline{\lambda}'S^-X'\underline{y}] + 0, \text{ since } \underline{\lambda}' = \underline{\lambda}'H \\
 &= \underline{\lambda}'S^-X'X\underline{\beta} = \underline{\lambda}'S^-S\underline{\beta} \\
 &= \underline{\lambda}'H\underline{\beta} \\
 &= \underline{\lambda}'\underline{\beta}.
 \end{aligned}$$

2. Unique: Let Rank (X) = r. Let it be possible to rearrange the columns of X with a corresponding rearrangement of the elements of $\underline{\beta}$ in such a manner that the first r columns of X, denoted X_1 , be independent. Partitioning X as $[X_1: X_2]$, we have

$$[X' X] \underline{\beta} = \begin{bmatrix} X_1' X_1 & X_1' X_2 \\ X_2' X_1 & X_2' X_2 \end{bmatrix} \underline{\beta} = S \underline{\beta} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} \underline{\beta}_r \\ \underline{\beta}_{p-r} \end{bmatrix} = \begin{bmatrix} X_1' \\ X_2' \end{bmatrix} \underline{y} = \begin{bmatrix} X_1' \underline{y} \\ X_2' \underline{y} \end{bmatrix}$$

where Rank (S_{11}) = r, $\underline{\beta}_r$ denotes the first r elements of $\underline{\beta}$, and $X_1' \underline{y}$, the first r elements of $X' \underline{y}$. Application of the "sweep-out" procedure would reduce the above equation to

$$\begin{bmatrix} S_{11} & S_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\underline{\beta}}_r \\ \hat{\underline{\beta}}_{p-r} \end{bmatrix} = \begin{bmatrix} X_1' \underline{y} \\ 0 \end{bmatrix}.$$

Applying the sweep-out procedure still further, we should have

$$\begin{bmatrix} I_r & S_{11}^{-1} S_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\underline{\beta}}_r \\ \hat{\underline{\beta}}_{p-r} \end{bmatrix} = \begin{bmatrix} S_{11}^{-1} (X_1' \underline{y}) \\ 0 \end{bmatrix}.$$

That is,

$$\begin{bmatrix} I_r & H_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\underline{\beta}}_r \\ \hat{\underline{\beta}}_{p-r} \end{bmatrix} = \begin{bmatrix} S_{11}^{-1} (X_1' \underline{y}) \\ 0 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} \hat{\underline{\beta}}_r \\ \hat{\underline{\beta}}_{p-r} \end{bmatrix} = \begin{bmatrix} S_{11}^{-1} (X_1' \underline{y}) \\ 0 \end{bmatrix} \quad (19)$$

Since $S_{11}^{-1} (X_1' \underline{y})$ is unique, the particular solution given in (19) is unique.

Hence, the estimate $\lambda' \hat{\beta}$ reduces to

$$\lambda' \hat{\beta} = \lambda' S^{-1} X' Y + \lambda' (I-H) Z = \lambda' S^{-1} X' Y$$

where $S^{-1} X' Y$ is the particular solution. The above reduces to $\lambda_r' S_{11}^{-1} (X_1' Y)$, where λ_r' represents the first r elements of λ' . $\lambda_r' S_{11}^{-1} (X_1' Y)$ is unique.

C. Variance of the Estimate $\lambda' \hat{\beta}$

$$\begin{aligned} V(\lambda' \hat{\beta}) &= V(\lambda' S^{-1} X' Y) \\ &= (\lambda' S^{-1} X' X S^{-1} \lambda) \sigma^2, \quad \text{since } (S^{-1})' = (S')^{-1} = S^{-1} \\ &= (\lambda' S^{-1} S S^{-1} \lambda) \sigma^2 = [\lambda' S^{-1} (\lambda' S^{-1} S)] \sigma^2 \\ &= [\lambda' S^{-1} (\lambda' H)] \sigma^2 = (\lambda' S^{-1} \lambda) \sigma^2. \end{aligned} \quad (20)$$

We have seen above that the estimate $\lambda' \hat{\beta}$ reduces to $(\lambda_r' S_{11}^{-1} X_1' Y)$. Hence, the variance of $\lambda' \hat{\beta}$ will reduce to

$$\begin{aligned} &[(\lambda_r' S_{11}^{-1} X_1') (\lambda_r' S_{11}^{-1} X_1')'] \sigma^2 \\ &= (\lambda_r' S_{11}^{-1} X_1' X_1 S_{11}^{-1} \lambda_r) \sigma^2 \\ &= (\lambda_r' S_{11}^{-1} \lambda_r) \sigma^2 \quad \text{which is unique.} \end{aligned}$$

D. On the Estimate $\hat{\sigma}^2$ Which is Unique and Unbiased

While the normal equations (16) will provide infinitely many solutions for $\hat{\beta}$, the estimate $\hat{\sigma}^2$ is unique, although it contains $\hat{\beta}$. $\hat{\sigma}^2$ is given by

$$\hat{\sigma}^2 = \frac{1}{n-r} [Y' Y - \hat{\beta}' X' Y] \quad (21)$$

In equation (21), $\hat{\beta}' X' Y = (Y' X) \hat{\beta}$ is unique, since $(Y' X) \hat{\beta}$ is of the form $\lambda' \hat{\beta}$, where λ' is a combination of the row vectors of X and thus

$\underline{\lambda}' \underline{\beta}$ is estimable with a unique estimate $\underline{\lambda}' \hat{\underline{\beta}} = (\underline{y}' X) (X' X)^{-1} X' \underline{y}$. Hence (21) reduces to

$$\begin{aligned} & \left(\frac{1}{n-r} \right) \underline{y}' [I - X S^{-1} X'] \underline{y} \\ &= \left(\frac{1}{n-r} \right) [X \underline{\beta} + \underline{\varepsilon}]' [I - X S^{-1} X'] [X \underline{\beta} + \underline{\varepsilon}] \\ &= \left(\frac{1}{n-r} \right) [\underline{\beta}' X' (I - X S^{-1} X') X \underline{\beta} + 2 \underline{\varepsilon}' (I - X S^{-1} X') X \underline{\beta} + \underline{\varepsilon}' (I - X S^{-1} X') \underline{\varepsilon}] \\ &= \left(\frac{1}{n-r} \right) [\underline{\beta}' (X' X - X' X S^{-1} X) \underline{\beta} + 2 \underline{\varepsilon}' (I - X S^{-1} X') X \underline{\beta} + \underline{\varepsilon}' (I - X S^{-1} X') \underline{\varepsilon}] \end{aligned}$$

The first component of the above expression is 0. If we take expectation of the remaining terms, the second term will be 0. The expectation of the third term which is a quadratic form in $\underline{\varepsilon}$ with mean 0 and variance $\sigma^2 I$ will be equal to (by a well known theorem, see [8]).

$$\begin{aligned} & \sigma^2 \text{Trace} [I - X S^{-1} X'] \\ &= \sigma^2 (n - \text{Trace} X S^{-1} X') \\ &= \sigma^2 (n - \text{Trace} S S^{-1}) = \sigma^2 (n - \text{Trace} H) \\ &= \sigma^2 (n-r) . \end{aligned}$$

Hence, the estimate $\hat{\sigma}^2$ is unbiased.

E. Scheffé's Theorem

Scheffé's theorem as given in (8) will reduce, when Rank (X) = r, to

$$\hat{\psi} - S \hat{\sigma}_{\psi} \leq \psi \leq \hat{\psi} + S \hat{\sigma}_{\psi} , \quad (22)$$

where $S^2 = [q F_{\alpha}; q, n-r]$, $q \leq r$. The change of (n-p) to (n-r) should be noted. It should also be noted that ψ is now of the form $\underline{\lambda}' \underline{\beta}$, where $\underline{\lambda}' = \underline{\lambda}' H$. In the light of what has been provided in this section, $\hat{\sigma}_{\psi}^2 = (\underline{\lambda}' S^{-1} \underline{\lambda}) \hat{\sigma}^2$.

In Design of Experiments, the function $\psi = \underline{\lambda}' \underline{\beta}$ is often required to be of the form of a contrast, and we may be interested in all possible contrasts which are mutually orthogonal.

A contrast among the parameters is defined to be a linear function of the parameters, $\sum_{i=1}^p c_i \beta_i$, such that $\sum_{i=1}^p c_i = 0$.

Two contrasts $\psi_1 = \sum_{i=1}^p c_i \beta_i$, $\psi_2 = \sum_{i=1}^p d_i \beta_i$ are said to be orthogonal, if and only if $\sum_{i=1}^p c_i d_i = 0$.

If we are interested in all possible contrasts which are mutually orthogonal, q will change to $(r-1)$, because we can only think of $(r-1)$ mutually orthogonal contrasts from a space of rank r .

If a set of q linear functions $\Lambda \underline{\beta}$, where Λ is of dimension $q \times p$, are individually estimable, their linear compound $\phi = \underline{\ell}' \Lambda \underline{\beta}$, where $\underline{\ell}$ is a $q \times 1$ column vector of constants, will also be estimable. The variance of $\hat{\phi}$ will be given by

$$\sigma_{\hat{\phi}}^2 = \sigma^2 [(\Lambda' \underline{\ell})' S^{-1} (\Lambda' \underline{\ell})]. \quad (23)$$

Hence, we may also have an analog of the formula given in (9).

It may be noted that if one is interested in contrasts of the type $(\beta_i - \beta_{i'})$, then one may use the confidence intervals given by Tukey (see Scheffé³ and Graybill⁸), as such intervals would give shorter lengths.

F. An Illustration

We provide below a simple example illustrating the use of Scheffé's theorem as given in (22). The example is drawn from an experiment in which it was desired to find the contributions of three factors represented by β_1 , β_2 and β_3 . $Y = X\beta$ is obtained as

$$X\beta = Y$$

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = \begin{bmatrix} 7.8 \\ 8.0 \\ 0.8 \\ 0.4 \end{bmatrix}$$

Measurements

The 4×3 design matrix X is of rank 2. Hence, $n = 4$, $r = 2$, $p = 3$. For the normal equations $S\hat{\beta} = X'Y$, we have

$$\begin{bmatrix} 4 & 0 & 2 \\ 0 & 4 & 2 \\ 2 & 2 & 2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \end{bmatrix} = \begin{bmatrix} 17.0 \\ 14.6 \\ 15.8 \end{bmatrix}$$

The first g-inverse of S is obtained as

$$S^- = B = \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix}, \quad \text{and } H = S^-S = \begin{bmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 \end{bmatrix}$$

The particular solution is obtained as

$$\hat{\beta} = B(X'Y) = \begin{bmatrix} 4.25 \\ 3.65 \\ 0 \end{bmatrix}$$

An estimable parametric function will obviously be given by $\lambda' = [1 \ 0 \ \frac{1}{2}]$, as it satisfied $\lambda' = \lambda' H$.

$$\text{Hence, } \lambda' \hat{\beta} = \begin{bmatrix} 1 & 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 4.25 \\ 3.65 \\ 0 \end{bmatrix} = 4.25 = \hat{\psi}.$$

Again, $\hat{\sigma}^2$ is estimated by

$$\begin{aligned} & \frac{1}{n-r} [Y'Y - \hat{\beta}'X'Y] \\ &= \frac{1}{2} [125.64 - 125.54] \\ &= .05. \end{aligned}$$

Taking $q = 2$ and $\alpha = .05$, we have $qF_{\alpha; q, n-r} = qF_{.05; 2, 2} = S^2 = 2 \times 19.00 = 38.00$, $S = 6.16$, and $\text{Var}(\hat{\psi}) = \text{Var}(\lambda' \hat{\beta}) = \sigma^2 \lambda_r' S_{11}^{-1} \lambda_r = \sigma^2/4$.

Substituting .05 for σ^2 , we have, for $\text{Var}(\lambda' \hat{\beta}) = .0125$. Hence the 95 percent confidence bounds are given by $[4.25 \pm 6.16 (.11)] \rightarrow (3.57, 4.93)$.

In the above, $\lambda' \beta$ is of the form $\beta_1 + \beta_3/2$. Depending on the necessity, we could also work with the estimable functions, such as $\beta_2 - \beta_1$, $\beta_1 + \beta_2 + \beta_3$, etc.

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